Structure Search in Cortellis
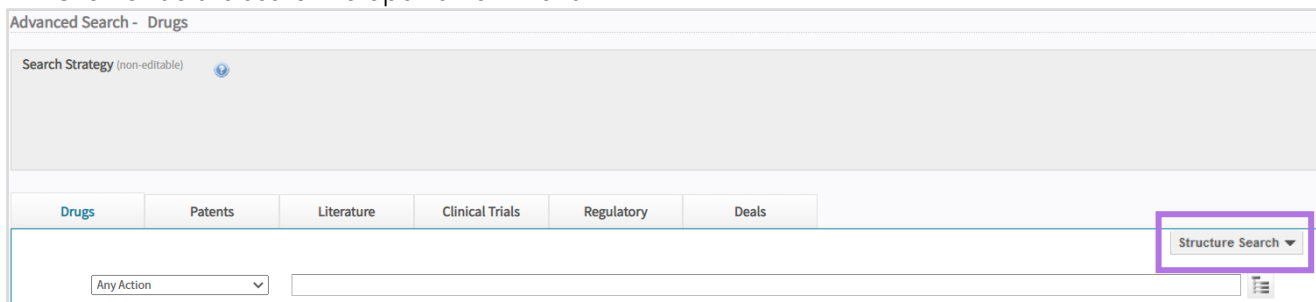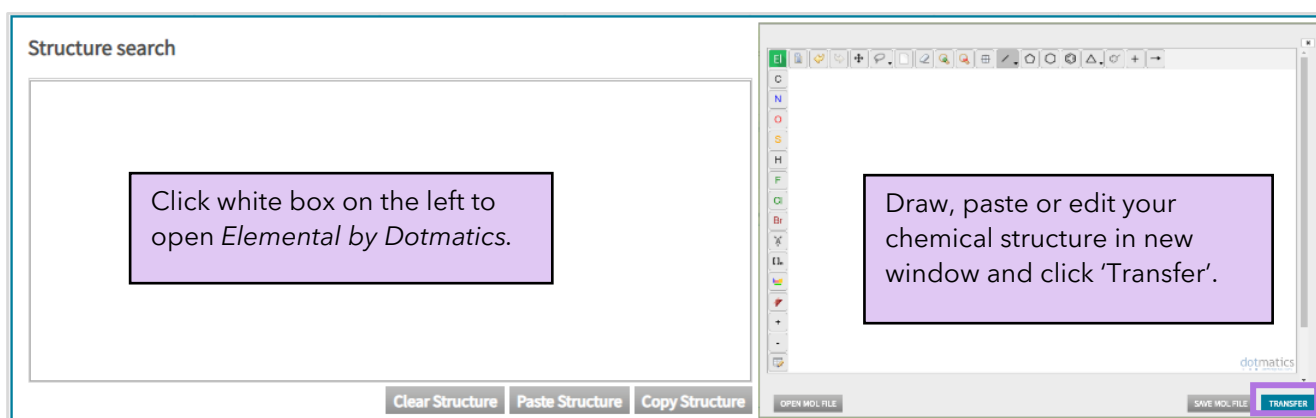
Structure Search is available from the "more" menu (…) in the main search bar as well as drugs, patents and literature forms in Advanced Search.

This guide provides instructions on how to find drugs according to their chemical structure in Cortellis **Advanced Search**.
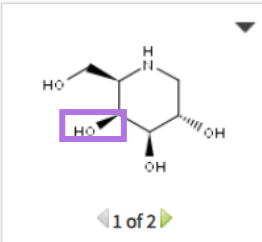
1. Click 'Structure search' to open a new menu.
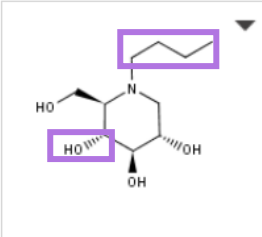

2. Structures can be transferred from reports and results tables in Cortellis, imported and drawn with *Elemental*.

Click white box on the left to open *Elemental by Dotmatics.*

Draw, paste or edit your chemical structure in new window and click 'Transfer'.

3. Select type of structure search, add additional fields to narrow down results and click 'Search' at the bottom right.
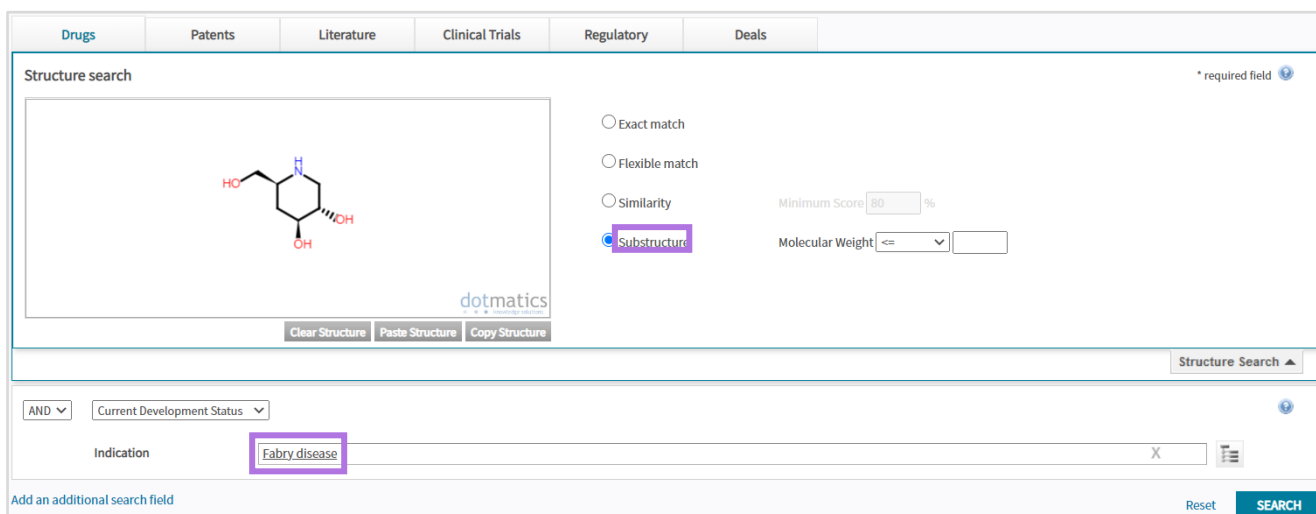
4. 'Hit structure' are displayed as a second column in results table. <u>Substructure</u> search will find drugs with same chirality and isomerism as in the original structure although these may have additional substituents, as indicated next.

Drug Name	Hit Structure	Originator Company	Active Companies	Highest Status
			Filters : [0]	Filters : [0]
migalastat	1 of 2	Mount Sinai School of Medicine	Amicus Therapeutics Inc	Launched
miglustat		GD Searle & Co	Johnson & Johnson; Teva Pharmaceutical Industries Ltd	Launched

Example: The next search will find drugs with <u>similar</u> chemical structures which means they may have other substituents, different chirality and/or different isomerism compared to the original structure.
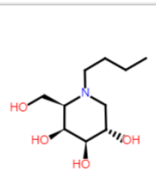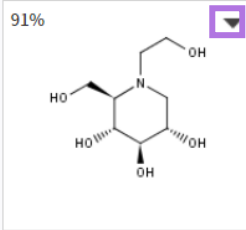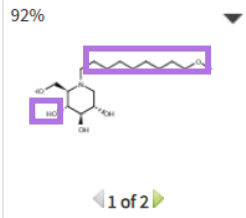

When running 'Similarity' search results table will automatically display percentage of similarity in the Hit Structure column.

Drug Name	Hit Structure	Originator Company	Active Companies	Active Indications
			Filters : [0]	Filters : [0]
miglitol	91%	Bayer AG	Pfizer Inc; Sanofi (pre-1999); Sanofi SA; Sanofi-Synthelabo; Sanwa Kagaku Kenkyusho Co	Non-insulin dependent diabetes
EBI-001	92% 1 of 2	University of Oxford	Emergent BioSolutions Inc	Viral infection

Structure can be saved, exported and transferred to other search forms in Cortellis by clicking the button at the top right.

Definitions

- **Exact match** retrieves all Drug Reports or Literature Reports or Patent Reports or Conference Presentations or containing a structure that matches your structure query exactly.

- **Flexible match** retrieves all Drug Reports or Literature Reports or Patent Reports or Conference Presentations containing a structure that matches your query structure exactly including stereoisomers, tautomers, salts of and charge variants.

- **Similarity** retrieves all Drug Reports or Literature Reports or Patent Reports or Conference Presentations containing structures that are similar to the query structure, based on the minimum percentage similarity score. The Minimum score is set initially at a value of 80%, but you can optionally specify a value between 0 and 100.

- **Substructure** retrieves all Drug Reports or Literature Reports or Patent Reports or Conference Presentations containing structures that match your query structure entirely or as a substructure within a larger structure. Substructure search is selected by default.

- Optional. **Specify molecular weight** to include only structures within a desired range; options are less than (<), more than (>), less than or equal to (<=), more than or equal to (>=), or between. Enter a number into the text box, e.g. <= 20.

Note: When using the similarity option, you should always enter the full structure that you want to find compounds similar to.

For more information contact Customer Service at **LSH.support@clarivate.com.**